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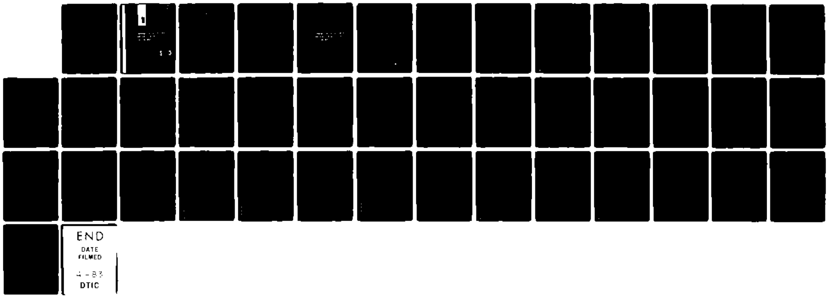

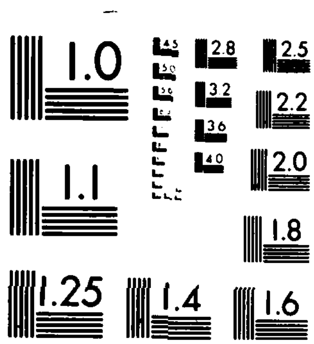

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Technical Memorandum

DIAGRAMS FOR THE FREE ENERGY AND DENSITY WEIGHT FACTORS OF THE ISING MODELS

R. A. FARRELL and S. FAVIN
The Johns Hopkins University Applied Physics Laboratory

P. H. E. MEIJER and P. ESFANDIARI
The Catholic University of America

THE JOHNS HOPKINS UNIVERSITY ■ APPLIED PHYSICS LABORATORY

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REPORT DOCUMENTATION PAGE

1. REPORT NUMBER: JHU/APL TG 1337 — 2. GOVT ACCESSION NO.: AD-A226 295	3. RECIPIENT'S CATALOG NUMBER
4. TITLE (and Subtitle): DIAGRAMS FOR THE FREE ENERGY AND DENSITY WEIGHT FACTORS OF THE ISING MODELS	5. TYPE OF REPORT & PERIOD COVERED: Technical Memorandum
	6. PERFORMING ORG. REPORT NUMBER: TG 1337
7. AUTHOR (s): R. A. Ferrell, S. Favin, P. H. E. Meijer, and P. Esfandiari	8. CONTRACT OR GRANT NUMBER (s): N00024-83-C-5301 N00014-78-C-0518
9. PERFORMING ORGANIZATION NAME & ADDRESS: The Johns Hopkins University Applied Physics Laboratory Johns Hopkins Road Laurel, MD 20707	10. PROGRAM ELEMENT, PROJECT, TASK AREA & WORK UNIT NUMBERS: X83J/RTP
11. CONTROLLING OFFICE NAME & ADDRESS: Naval Sea Systems Command Washington, D.C. 20362	12. REPORT DATE: January 1983
	13. NUMBER OF PAGES: 42
14. MONITORING AGENCY NAME & ADDRESS: Naval Plant Representative Office Johns Hopkins Road Laurel, MD 20707	15. SECURITY CLASS. (of this report): Unclassified
	15a. DECLASSIFICATION/DOWNGRADING SCHEDULE
16. DISTRIBUTION STATEMENT (of this Report): Approved for public release; distribution unlimited.	
17. DISTRIBUTION STATEMENT (of the abstract entered in Block 20, if different from Report)	
18. SUPPLEMENTARY NOTES	

19. KEY WORDS (Continue on reverse side if necessary and identify by block number)

diagrammatic expansion
Ising models
phase transitions
statistical mechanics

20. ABSTRACT (Continue on reverse side if necessary and identify by block number)

This report describes the evaluation of the free energy of the nearest neighbor Ising model through tenth order in the inverse temperature variable (J/kT). The free energy is expressed in terms of diagrams composed of interaction bonds and vertices. An explicit list of the diagrams with 10 or fewer bonds is presented, and the unrestricted lattice constants (free multiplicities) of these diagrams are given for the cubic lattices. We employ a theorem that states that a certain sum of diagrams is zero in order to obtain the density-dependent weight factors associated with the vertices. These factors are polynomials in the density and depend on the kind of articulated vertex under consideration. Explicit denumeration of the diagrams is given for those articulated vertices of the fourth and fifth kind that are needed in the tenth order expansion. These methods reproduce the known results for the cubic lattices.

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The work described in this report was performed under U.S. Navy contracts N00024-83-C-5301 (The Johns Hopkins University Applied Physics Laboratory) and N00014-78-C-0518 (The Catholic University).

JHU/APL
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R. A. FARRELL and S. FAVIN
The Johns Hopkins University Applied Physics Laboratory

P. H. E. MEIJER and P. ESFANDIARI *
The Catholic University of America

***Currently at Vitro Laboratories, Automation Industries, Silver Spring, Md.**

THE JOHNS HOPKINS UNIVERSITY ■ APPLIED PHYSICS LABORATORY
Johns Hopkins Road, Laurel, Maryland 20707
Operating under Contract N00024-83-C-5301 with the Department of the Navy

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This report describes the evaluation of the free energy of the nearest neighbor Ising model through tenth order in the inverse temperature variable (J/kT). The free energy is expressed in terms of diagrams composed of interaction bonds and vertices. An explicit list of the diagrams with 10 or fewer bonds is presented, and the unrestricted lattice constants (free multiplicities) of these diagrams are given for the cubic lattices. We employ a theorem that states that a certain sum of diagrams is zero in order to obtain the density-dependent weight factors associated with the vertices. These factors are polynomials in the density and depend on the kind of articulated vertex under consideration. Explicit denumeration of the diagrams is given for those articulated vertices of the fourth and fifth kind that are needed in the tenth order expansion. These methods reproduce the known results for the cubic lattices.

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1. INTRODUCTION

The exact solution to the free energy of the three-dimensional Ising model is not known, but exact series expansions have proven quite beneficial for deducing the thermodynamic properties of these systems.[1-6] The terms in these series are evaluated through some order in an expansion variable, and diagrammatic methods are a valuable aid for cataloging the various contributions. The steps involved in obtaining such expansions are: (1) list the topologically distinct diagrams, (2) generate the weight factors that are associated with the vertices of the diagram, and (3) calculate the appropriate lattice constant (the number of ways the diagram can be embedded in the lattice). The degree of difficulty of these steps, as well as the need to make modifications appropriate to the particular model (e.g., particular lattice or particular interaction potential), depend on the specific diagrammatic expansion. The present report uses an especially convenient expansion to analyze nearest-neighbor models on cubic lattices; application to other systems can be achieved by calculating the unrestricted lattice constants (i.e., free multiplicities) for them.

---

[1] *Phase Transitions and Critical Phenomena* Vol. 3, C. Domb and M. S. Green (eds.), Academic Press, London (1974).

[2] M. F. Sykes, D. S. Gaunt, P. D. Roberts, and J. A. Wyles, "High Temperature Series for the Susceptibility of the Ising Model; I. Two Dimensional Lattices, and II. Three Dimensional Lattices," *J. Phys. A* **5**, 6, 640 (1972).

[3] M. F. Sykes, D. L. Hunter, D. S. McKenzie, and B. R. Heap, "Specific Heat of a Three Dimensional Ising Ferromagnet above the Curie Temperature II," *J. Phys. A* **5**, 667 (1972).

[4] P. H. E. Meijer and R. A. Farrell, "Padé Approximations and the Critical Exponents in the Two-and Three-Dimensional Ising Models," *Phys. Rev. B* **12**, 3 (1975).

[5] D. S. Gaunt and G. A. Baker, Jr., "Low-temperature Critical Exponents from High-temperature Series: The Ising Model," *Phys. Rev. B* **1**, 1184 (1970)

[6] G. Paul and H. E. Stanley, "Partial Test of the University Hypothesis: The Case of Next-Nearest-Neighbor Interactions," *Phys. Rev. B* **5**, 3715 (1972).

2. FREE ENERGY

The Helmholtz free energy, F, of the Ising model can be written[7,8] as

$$-\beta F = -L[\rho \ell n \rho + (1-\rho)\ell n(1-\rho)] + \sum_{Sites} \sum_{D'} D' , \quad (1)$$

where β is the usual Boltzmann temperature factor, $1/(kT)$; ρ is the density (fraction of sites that are occupied), and D' is the set of topologically distinct connected diagrams composed of interaction bonds and density dependent vertices. Any number of bonds can connect sites i and j; the weight to be assigned such a bond is $(\beta J_{i,j})$ if $i \neq j$ and 0 if $i = j$, where $J_{i,j}$ is the interaction energy between particles on these sites. The weight factor associated with a vertex is a polynomial in the density whose coefficients depend on the "kind of articulation vertex" that is under consideration. An articulation vertex is of the pth kind (or order) if its removal would cause the diagram to separate into p disjoint parts. The simplest example of an articulation vertex is the central vertex in a star diagram composed of dumbbells that are joined at (or share) a common vertex (see Fig. 1). Such a vertex is of the sth kind if there are s points to the star.

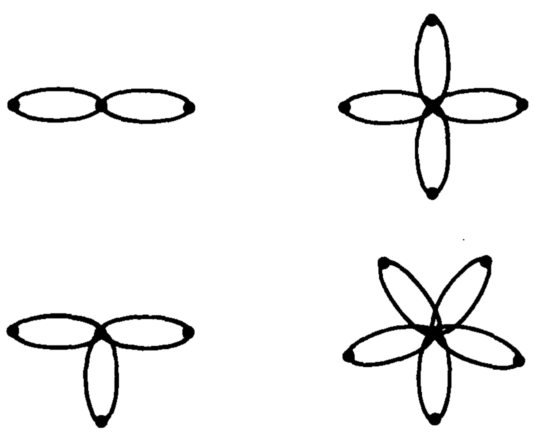


Figure 1—Simple examples of diagrams with articulated vertices: $\nu > 1$.

The usual virial expansion of the free energy involves the sum of more than singly connected single-bonded diagrams composed of vertices having weight ρ interconnected by bonds $b_{i,j}$ and $-\delta_{i,j}$. Here, single-bonded means that no more than one bond can connect a pair of vertices; $b_{i,j} = [\exp(\beta J_{i,j}) - 1]$; and $\delta_{i,j}$ is 1 if $i = j$, and is 0 if $i \neq j$. Equation 1 is obtained[7,9] by: (1) Taylor series expanding the factor $[\exp(\beta J_{i,j}) - 1]$, which leads to multiple $(\beta J_{i,j})$-bonds and a symmetry factor to account for the interchangeability of the multiple bonds that connect a pair of vertices; (2) using the well-known result for the hard core gas to evaluate the sum of diagrams that do not contain $(\beta J_{i,j})$-bonds; (3) demonstrating that there is an exact cancellation among the set of diagrams that contain $b_{i,j}$-bonds and have one or more vertices that do not have at least one $b_{i,j}$-bond emanating from them; and (4) introducing density weight factors to accomplish a vertex renormalization, i.e., to sum over $-\delta_{i,j}$-bond configurations. The density weight factor for an articulation vertex of the νth kind is denoted by $M_{n_1,n_2,\ldots,n_\nu}$, where n_i is the number of bonds that connect the vertex to the ith disjoint part into which the diagram would separate if the vertex were removed. Step 3 demonstrates that each vertex, ρ, has one or more $b_{i,j}$ bonds emanating from it, so that the weight factor is a polynomial in the density of order of the number of bonds emanating from the circle, i.e., of order $\sum_{i=1}^{\nu} n_i$.

The density weight factor for articulation vertices of the first, second, and third kind have been obtained[8] from recurrence relations among their coefficients. A detailed description of the derivation of the recurrence relations is given in Ref. 7. The generating functions that lead to these relationships are a direct consequence of a diagrammatic theorem[7] that expresses the density weight factors for vertices of higher kind in terms of sums of products of density weight factors of lower kinds. This theorem, or zero sum rule, states that the contribution of the diagram representing $M_{n_1,n_2,\ldots,n_\nu}$ plus the contributions of all its associated diagrams sum to zero. The associated

[7] R. A. Farrell, T. Morita, and P. H. E. Meijer, "Cluster Expansion for the Ising Model," *J. Chem. Phys.* **45**, 349 (1966).

[8] P. Esfandiari, P. H. E. Meijer, R. A. Farrell, and S. Favin, "New Generating Functions and Results for the Density Polynomials of the Lattice Gas," *Phys. Rev. B* **24**, 1298 (1981), also, "Erratum: New Generating Functions and Results for the Density Polynomials of the Lattice Gas," *Phys. Rev. B* **25**, 6030 (1982).

[9] T. Morita and K. Hiroike, "A New Approach to the Theory of Classical Fluids, III — General Treatment of Clasical Systems," *Prog. Theor. Phys.* **25**, 537 (1961)

diagrams are constructed as follows. The ν disjoint parts into which the diagram would separate if this circle were removed are represented by ν labeled black triangles on a field (compare Fig. 2). Open p-gons ($p = 2$ is a circle, $p = 3$ a triangle, etc.) are inserted between the black triangles in all possible combinations. Inside each p-gon are one or more black dots that are connected to the black triangles by bonds of weight 1. The following three rules must be obeyed: (1) each black triangle is not articulated, and black triangle i has exactly n_i bonds emanating from it, (2) each black dot within a given p-gon is connected to p specific black triangles, and (3) the number of black dots within a p-gon is only restricted by the constraint that it obey these rules.

This classification is trivial for $\nu = 2$, and for $\nu = 3$ it generates the five types of diagrams shown in Fig. 2. The evaluation of these generic diagrams produces the generating functions given in Ref. 7. We have used analogous classifications to construct the sets of associated diagrams for each of the density weight factors of the fourth and fifth kind needed to calculate the free energy through tenth order in inverse temperature. The use of specific n_i's simplifies the procedure by eliminating certain generic diagrams that would occur for larger n_i's. In order to illustrate this simplification, consider what would happen if we had listed the associated diagrams for the $\nu = 3$ case of $M_{2,2,2}$. Because only two bonds would emanate from each star, neither the second nor the third types of generic diagrams in Fig. 2 would appear in the list. Analogous exclusions occur for $\nu = 4$ and 5. In Ref. 7, the procedure was illustrated by listing the diagrams for the case of $M_{2,2,2,2,2}$. In this report, we list all of the required diagrams in Figs. 3 through 7. From these figures and the generating functions derived in Ref. 7, one obtains the density weight factors listed in Table 1.

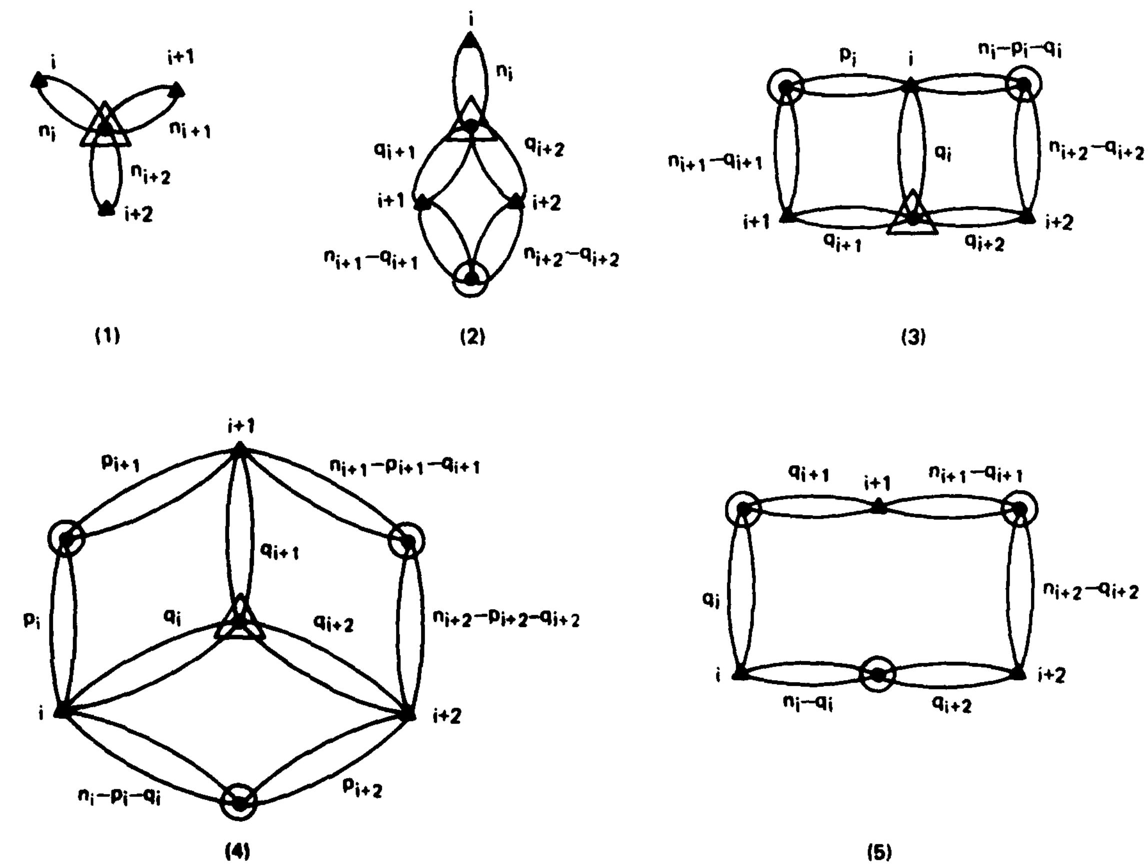


Figure 2—The five generic diagrams generated by the $\nu = 3$ sum rule.

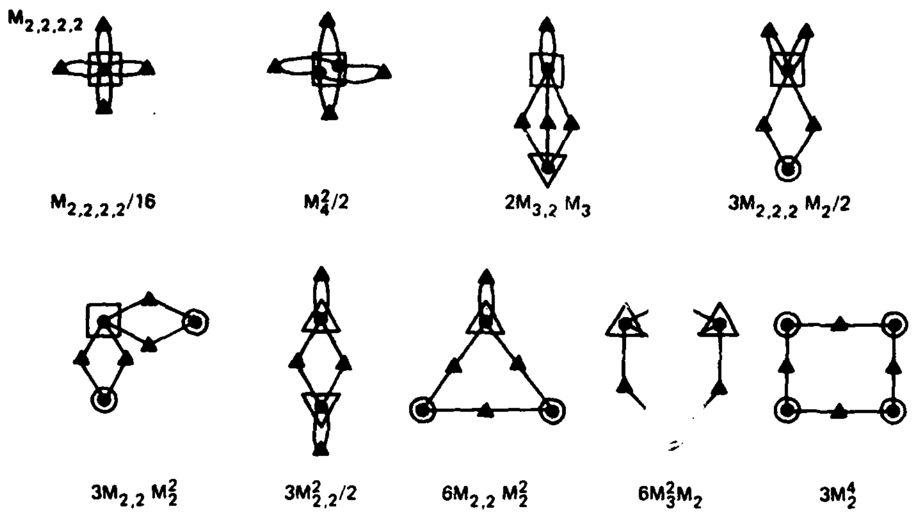


Figure 3—The diagrams that contribute to $M_{2,2,2,2}$.

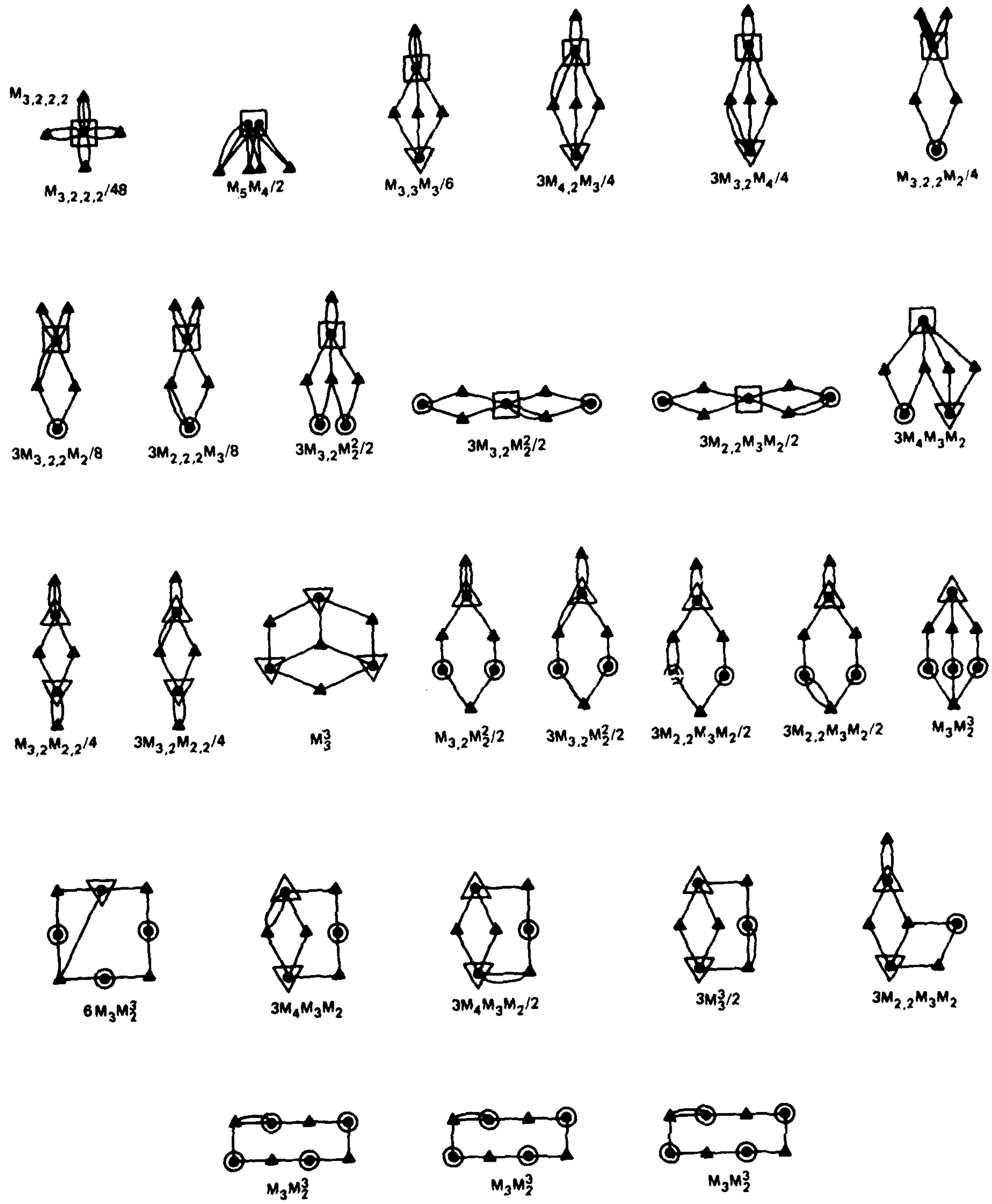
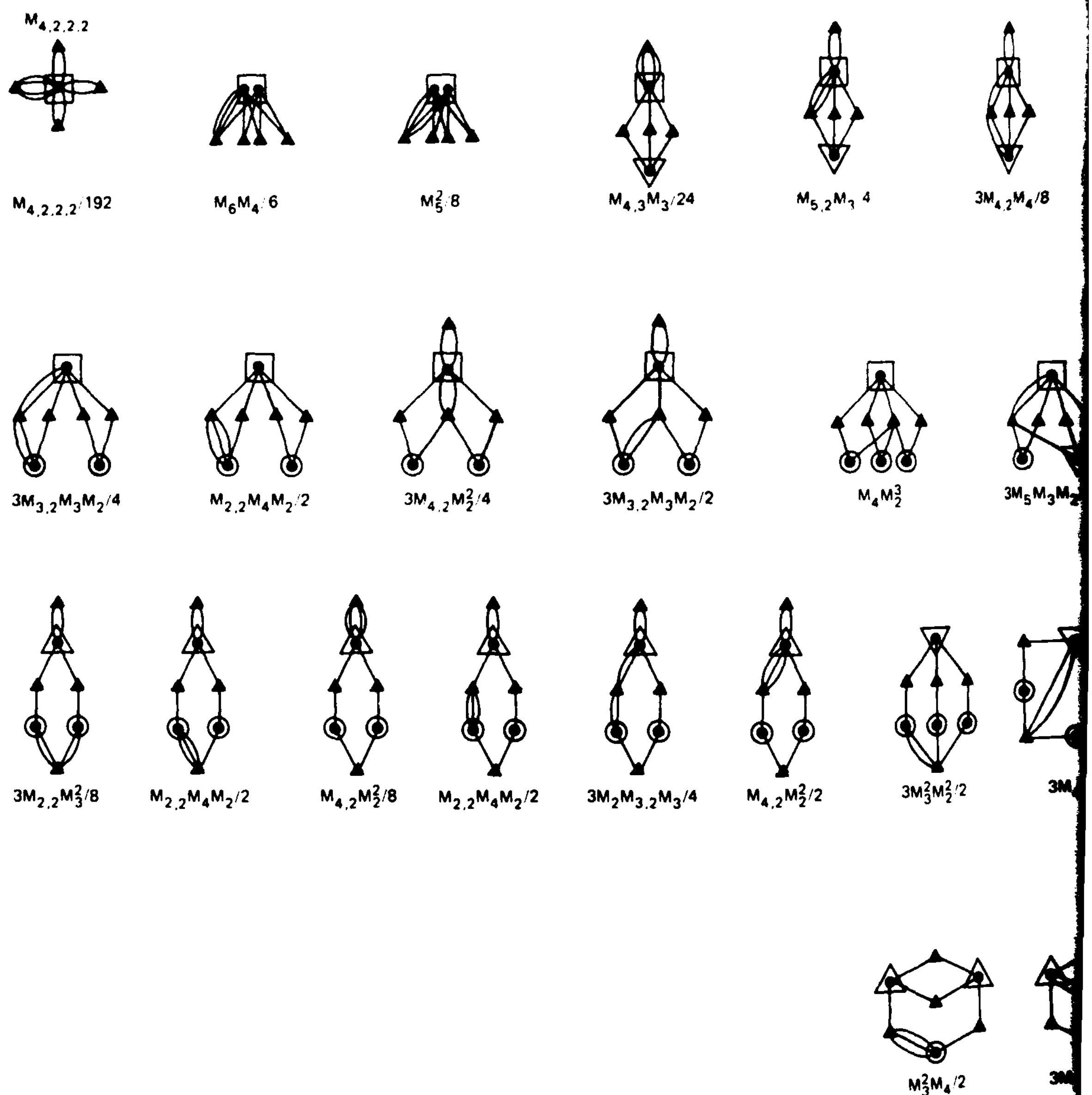


Figure 4—The diagrams that contribute to $M_{3,2,2,2}$.


$M_{4,2,2,2}$
$M_{4,2,2,2}/192$
$M_6M_4/6$
$M_5^2/8$
$M_{4,3}M_3/24$
$M_{5,2}M_3/4$
$3M_{4,2}M_4/8$
$3M_{3,2}M_3M_2/4$
$M_{2,2}M_4M_2/2$
$3M_{4,2}M_2^2/4$
$3M_{3,2}M_3M_2/2$
$M_4M_2^3$
$3M_5M_3M_2$
$3M_{2,2}M_3^2/8$
$M_{2,2}M_4M_2/2$
$M_{4,2}M_2^2/8$
$M_{2,2}M_4M_2/2$
$3M_2M_{3,2}M_3/4$
$M_{4,2}M_2^2/2$
$3M_3^2M_2^2/2$
$M_3^2M_4/2$

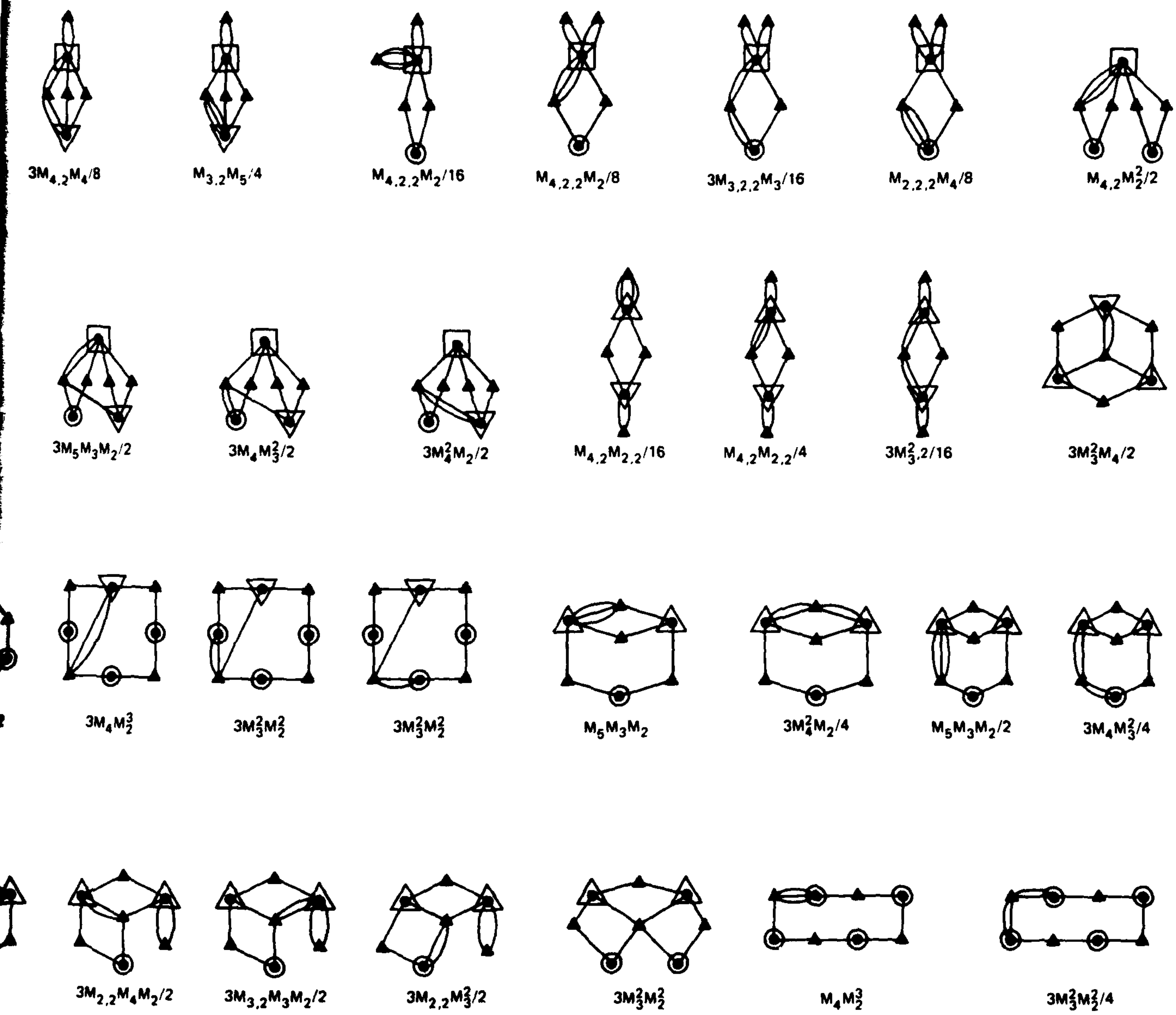
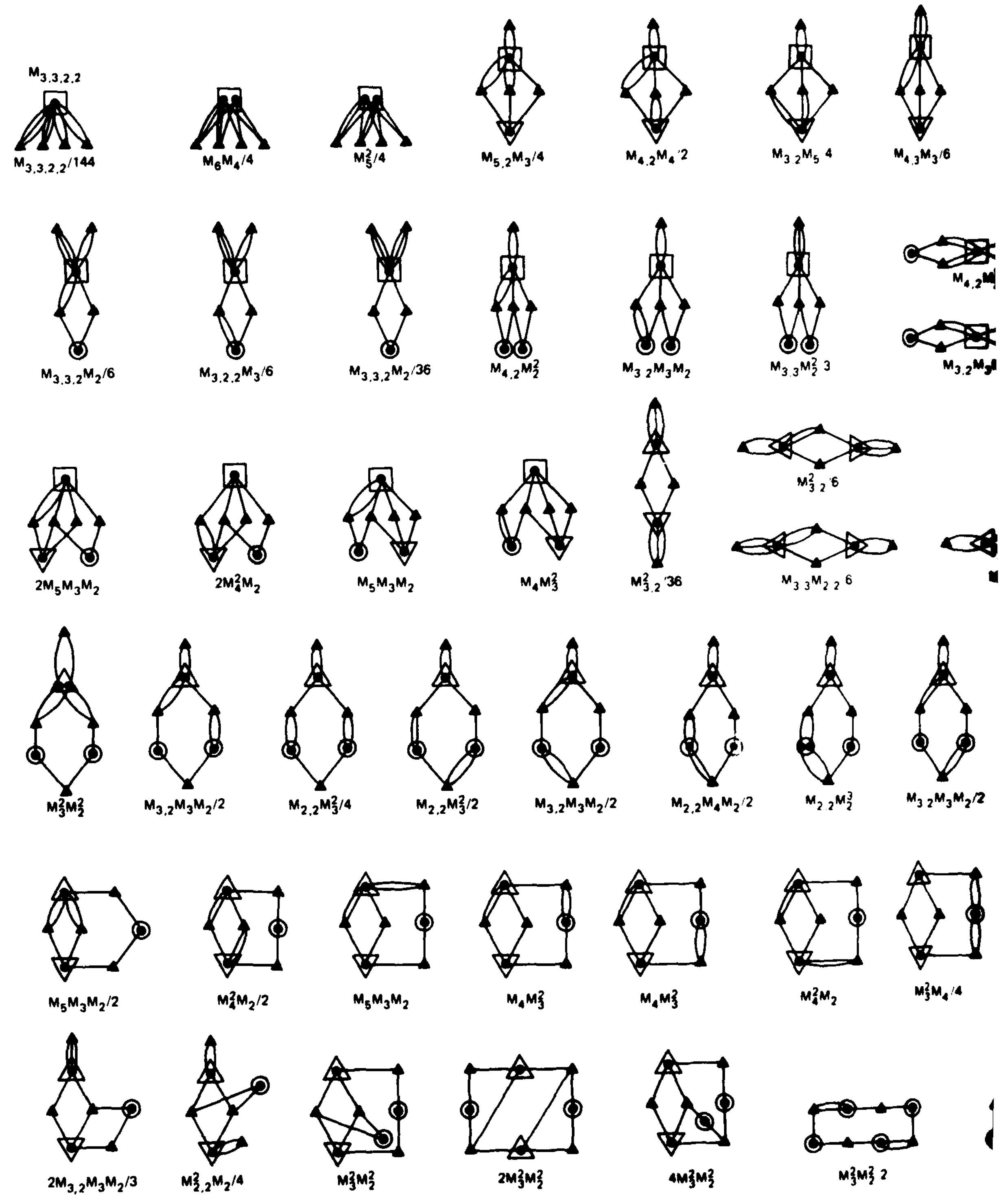


Figure 5—The diagrams that contribute to $M_{4,2,2,2}$.


$M_{3,3,2,2}$
$M_{3,3,2,2}/144$
$M_6M_4/4$
$M_5^2/4$
$M_{5,2}M_3/4$
$M_{4,2}M_4/2$
$M_{3,2}M_5/4$
$M_{4,3}M_3/6$
$M_{3,3,2}M_2/6$
$M_{3,2,2}M_3/6$
$M_{3,3,2}M_2/36$
$M_{4,2}M_2^2$
$M_{3,2}M_3M_2$
$M_{3,3}M_2^2/3$
$M_{3,2}^2/6$
$2M_5M_3M_2$
$2M_4^2M_2$
$M_5M_3M_2$
$M_4M_3^2$
$M_{3,2}^2/36$
$M_{3,3}M_{2,2}/6$
$M_3^2M_2^2$
$M_{3,2}M_3M_2/2$
$M_{2,2}M_3^2/4$
$M_{2,2}M_3^2/2$
$M_{3,2}M_3M_2/2$
$M_{2,2}M_4M_2/2$
$M_{2,2}M_2^3$
$M_{3,2}M_3M_2/2$
$M_5M_3M_2/2$
$M_4^2M_2/2$
$M_5M_3M_2$
$M_4M_3^2$
$M_4M_3^2$
$M_4^2M_2$
$M_3^2M_4/4$
$2M_{3,2}M_3M_2/3$
$M_{2,2}^2M_2/4$
$M_3^2M_2^2$
$2M_3^2M_2^2$
$4M_3^2M_2^2$
$M_3^2M_2^2/2$

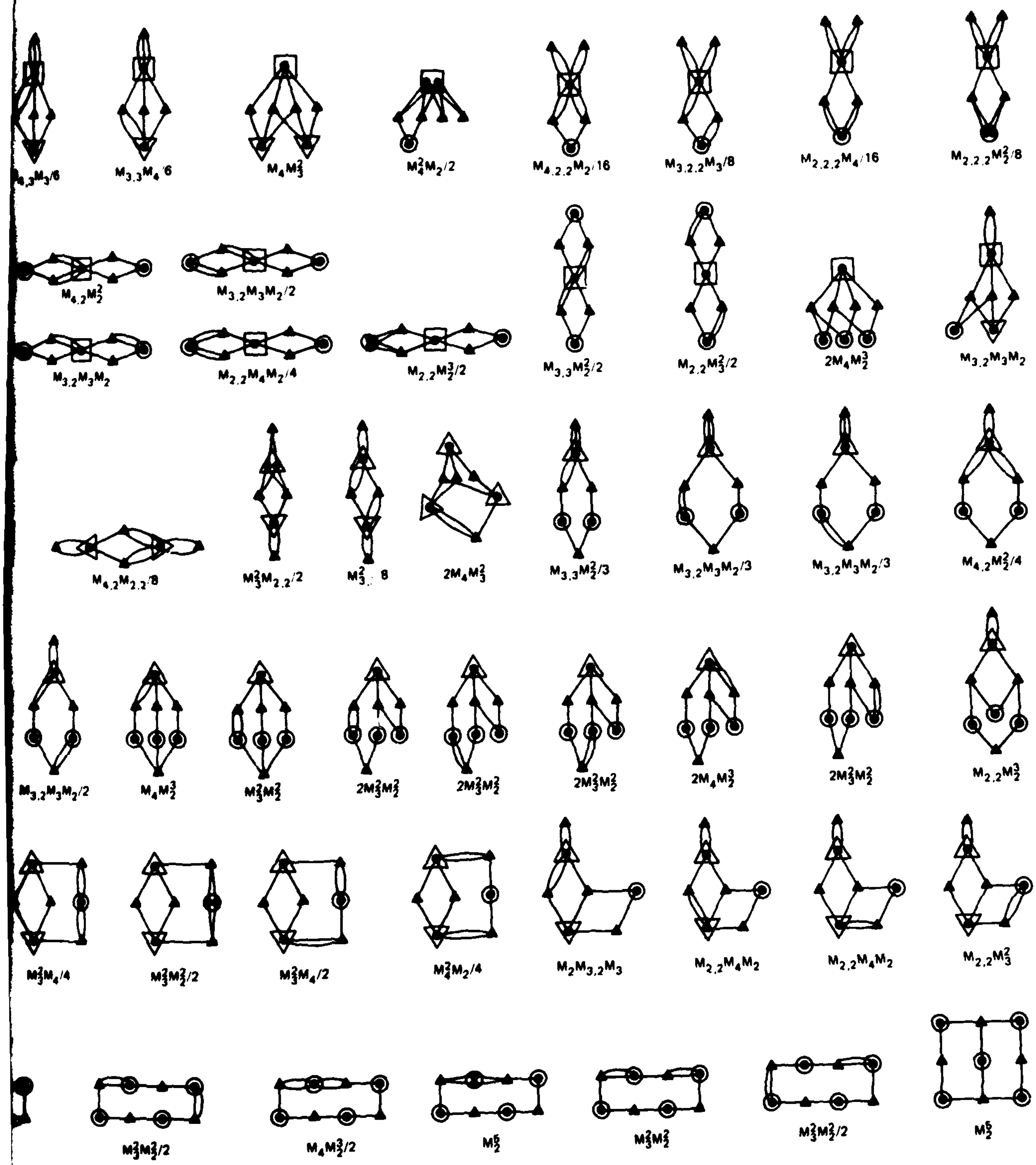


Figure 6—The diagrams that contribute to $M_{3,3,2,2}$.

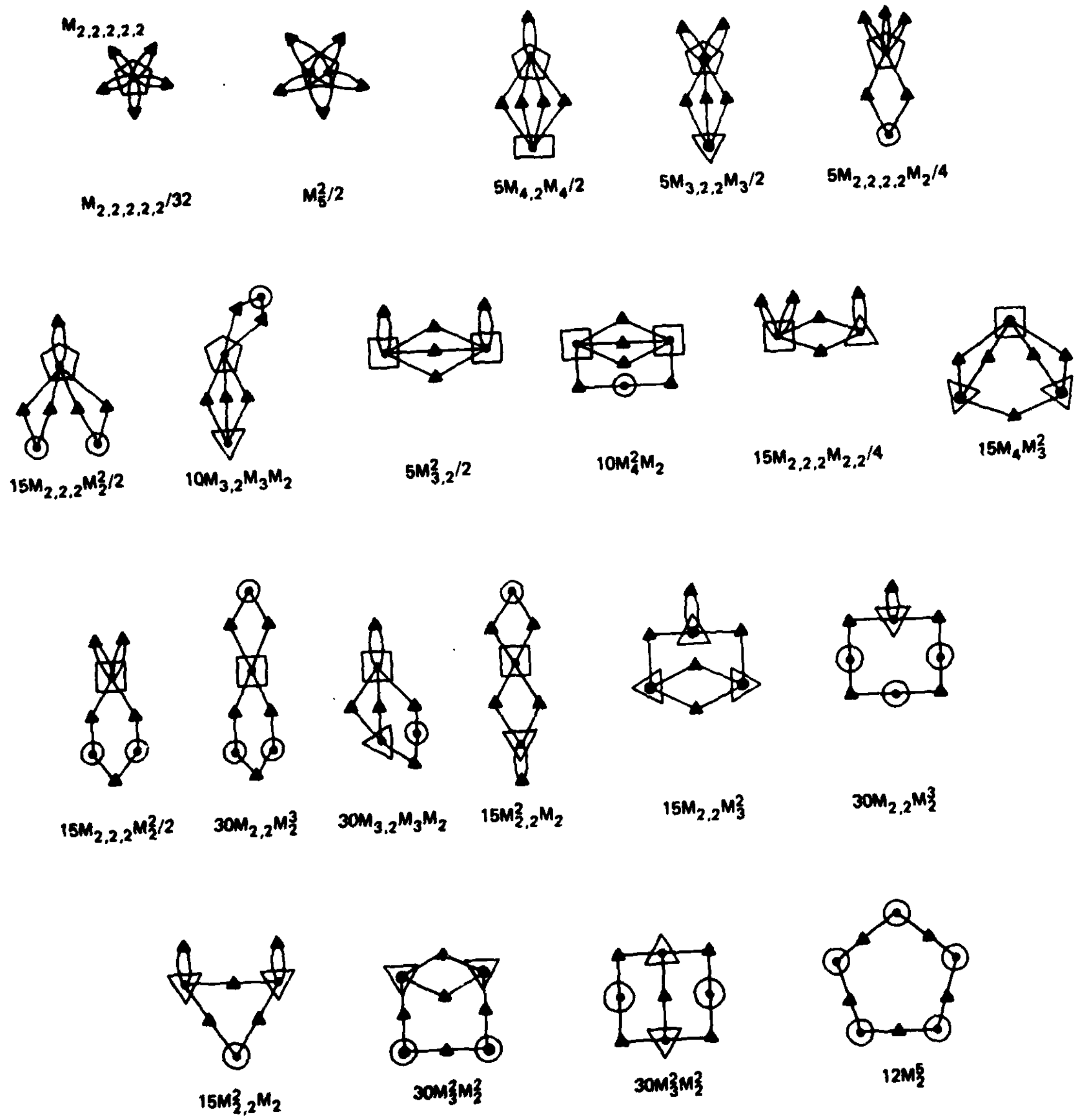


Figure 7—The diagrams that contribute to $M_{2,2,2,2,2}$.

Table 1—The coefficients $W_{n_1,n_2,\ldots,n_\nu,m}$ in

1	0	0	0	0	1	0	0	0
2	0	0	0	0	1	-1	0	0
3	0	0	0	0	1	-3	2	0
4	0	0	0	0	1	-7	12	-6
5	0	0	0	0	1	-15	50	-60
6	0	0	0	0	1	-31	180	-390
					-120	0	0	0
7	0	0	0	0	1	-63	602	-2100
					-2520	720	0	0
8	0	0	0	0	1	-127	1932	-10206
					-31920	20160	-5040	0
9	0	0	0	0	1	-255	6050	-46620
					-317520	332640	-181440	40320
10	0	0	0	0	1	-511	18660	-204630
					-2739240	4233600	-3780000	1814400
2	2	0	0	0	0	-2	4	-2
3	2	0	0	0	0	-6	24	-30
3	3	0	0	0	0	-18	120	-270
					-84	0	0	0
4	2	0	0	0	0	-14	100	-230
					-72	0	0	0
4	3	0	0	0	0	-42	456	-1650
					-2016	576	0	0
4	4	0	0	0	0	-98	1636	-6882
					-28224	17856	-4464	0
5	2	0	0	0	0	-30	360	-1350
					-1680	480	0	0
5	3	0	0	0	0	-90	1560	-8550
					-27300	17280	-4320	0
5	4	0	0	0	0	-210	5400	-42570
					-294000	308640	-168480	37440
5	5	0	0	0	0	-450	17400	-193950
					-2622900	4060800	-3628800	1742400
6	2	0	0	0	0	-62	1204	-6902
					-22680	14400	-3600	[illegible]
6	3	0	0	0	0	-186	5064	-4053
					-282240	296640	-162000	3600
6	4	0	0	0	0	-434	17140	-19181
					-2599632	4026240	-3598560	17280
7	2	0	0	0	0	-126	3864	-3259
					-235200	248640	-136080	302
7	3	0	0	0	0	-378	15960	-1820
					-2494884	3870720	-3462480	16632
8	2	0	0	0	0	-254	12100	-1459
					-2088072	3265920	-2933280	14112

ts $W_{n_1,n_2,\dots,n_\nu;m}$ in the density weight factor polynomial $M_{n_1,n_2,\dots,n_\nu} = \sum_{m=1}^{n_1+n_2+\dots n_\nu} W_{n_1,n_2,\dots n_\nu;m}\,\rho^m$.

0	0
0	0
0	0
-6	0
-60	24
-390 0	360 0
-2100 0	3360 0
-10206 0	25200 0
-46620 40320	166824 0
-204630 1814400	1020600 -362880

-2	0
-30	12
-270 0	252 0
-230 0	216 0
-1650 0	2676 0
-8882 0	22176 0
-1350 0	2220 0
-8550 0	21420 0
-42570 37440	153780 0
-193950 1742400	973980 -348480
-6902 0	17640 0
-40530 36000	147252 0
-191810 1728000	964656 -345600
-32550 30240	121212 0
-182070 1663200	922572 -332640
-145910 1411200	760536 -282240

2	2	2	0	0	0 -32	-4 0	40 0	-100 0	96 0
3	2	2	0	0	0 -1008	-12 288	192 0	-780 0	1320 0
3	3	2	0	0	0 -17640	-36 11232	864 -2808	-5220 0	13608 0
3	3	3	0	0	0 -229824	-108 242784	3744 -132840	-31860 29520	118584 0
4	2	2	0	0	0 -15344	-28 9792	712 -2448	-4444 0	11760 0
4	3	2	0	0	0 -200592	-84 212832	3072 -116640	-27060 25920	102552 0
4	3	3	0	0	0 -2191896	-252 3417120	12960 -3063960	-155340 1473120	802872 -294624
4	4	2	0	0	0 -1916768	-196 3006720	10600 -2704320	-131620 1301760	694176 -260352
5	2	2	0	0	0 -169680	-60 180960	2400 -99360	-22140 22080	85800 0
5	3	2	0	0	0 -1862280	-180 2924640	10080 -2631960	-126900 1267200	672840 -253440
6	2	2	0	0	0 -1566992	-124 2479680	7720 -2239920	-102460 1080000	558096 -216000
2	2	2	2	0	0 -8064	-8 5184	304 -1296	-2168 0	6048 0
3	2	2	2	0	0 -112896	-24 121536	1344 -66960	-13800 14880	55920 0
3	3	2	2	0	0 -1297296	-72 2064960	5760 -1870560	-81720 902880	456624 -180576
4	2	2	2	0	0 -1135008	-56 1817280	4720 -1650960	-69320 797760	395136 -159552
2	2	2	2	2	0 -656768	-16 1071360	2080 -982080	-35920 476160	220416 -95232

3. APPLICATION TO THE NEAREST NEIGHBOR MODEL

In order to determine the free energy we constructed two sets of lattice diagrams. The first set consists of all connected and nonarticulated diagrams that have 10 or fewer bonds. There are 185 single-bonded diagrams of this type; they are listed in Fig. 8, together with their symmetry numbers. The free multiplicities of these diagrams for nearest-neighbor models on the cubic lattices are presented in Tables 2 and 3. They are in accord with the recently published tables of Kincaid, Baker, and Fullerton.[10] The exclusion of triangular, pentangular, etc. figures on the simple-cubic and body-centered-cubic lattices greatly reduces the number of diagrams needed for those cases.

The second set of lattice diagrams consists of all the articulated diagrams with 10 or fewer bonds. These are generated by joining together two or more nonarticulated diagrams at one or more common vertices. In constructing these diagrams, one uses all the previously listed nonarticulated diagrams except that the single-bonded two-vertex diagram (i.e., the single-bonded dumbbell) cannot occur as an element emanating from a vertex; such a diagram element has to be at least double-bonded. This exclusion is a consequence of the fact that the articulation vertices are formed by collapsing a number of vertices (that were connected by $-\delta_{i,j}$-bonds). Subject to this restriction, we find that there are 245 topologically distinct articulated diagrams with the minimum number of bonds between their vertices; they are listed in Fig. 9, together with their symmetry numbers. The free multiplicity of an articulated diagram is simply the product of the free multiplicities of the nonarticulated diagram elements used to generate it; it has not been listed.

After these lists were composed and checked, we generated the additional terms by multiple-bonding all of the previously listed diagrams. Multiple-bonding does not change the number of ways the diagram fits into the lattice (i.e., its free multiplicity) but it does change the density weight factors, the order of the temperature contribution, and the symmetry number appropriate to the diagram. Multiple-bonding changes the symmetry of a diagram for two reasons. First, multiple-bonds that connect a given pair of vertices are equivalent; this is accounted for by introducing a product of factorials in recognition of their interchangeability. The second reason is that the overall symmetry of the single-bonded diagram can be changed. For example, the symmetry number of a p-gon is $2p$ because there are p rotations and one flip of the diagram, each of which leads to a diagram that is topologically equivalent. If one of the pairs of connected points in a p-gon is joined by multiple bonds and the other $(p-1)$ connections are single-bonded, then the symmetry number is reduced to 2 because the rotations lead to topologically distinct diagrams; only the flip around the center of the multiple bonded pair leads to a topologically equivalent diagram. Usually one would account for this change of symmetry by listing only topologically distinct unlabeled diagrams and using their modified symmetry numbers. Alternatively, one can sum over all possible multiple bondings of the single-bonded diagram independently and use the overall symmetry number of the single-bonded diagram (modified by the product of factorials mentioned above). We have used this alternative because it is ideally suited for a computing machine. This procedure is based on the fact that independent multiple-bonding can lead to topologically equivalent diagrams, and the number of such diagrams of a given type is simply the ratio of the symmetry number of the single-bonded diagram to that of the multiple bonded diagram. A few simple examples are presented in Fig. 10.

We created the computer compilation program reproduced and annotated in the appendix in order to accumulate the contributions of the aforementioned 430 lattice diagrams and the needed multiple-bonded diagrams that they generate. The following information is used to characterize each diagram: an arbitrary label, 1 to 430; the symmetry number of the single-bonded diagram; the unrestricted lattice constant (i.e., free multiplicity) for the lattice under consideration; the total number of vertices, NC; the total number of bonds (actually, the number of connected pairs of vertices), NB, in the single-bonded diagram; and two sequences of numbers to specify the diagram's topology (i.e., the manner in which the vertices are interconnected). The first sequence gives the lower limits on the number of bonds between each of the NB pairs of vertices that are connected. These numbers are in general equal to unity, except in the case of a two-vertex element (dumbbell) in an articulated diagram where the number is 2 (for the reasons discussed above). The second sequence of numbers consists of two subsets. The first subset

[10] J. M. Kinkaid, G. A. Baker, Jr., and L. W. Fullerton, "High-Temperature Series Expansions of the Continuous-Spin Ising Model," Los Alamos Scientific Report La-Ur-79-1575 (unpublished).

specifies the articulation order of each of the NC vertices; i.e., it is a sequence of NC numbers that are unity if the vertex is nonarticulated, 2 if the articulation is of the second kind, etc. The second subset gives the emanation numbers of each vertex. If the vertex is nonarticulated, there is only one set of emanation numbers that specify the other vertices to which it is connected. If it is an articulation vertex of the pth kind, there are p sets of emanation numbers needed because the diagram separates into p elements if the vertex is removed. In this case, each set of emanation numbers specifies those vertices within a particular one of the p elements that are connected to the vertex of interest. This scheme, cumbersome as it may seem, is a very efficient way to transfer the information into the code. The data were proofread several times and were checked by using them to regenerate the diagram.

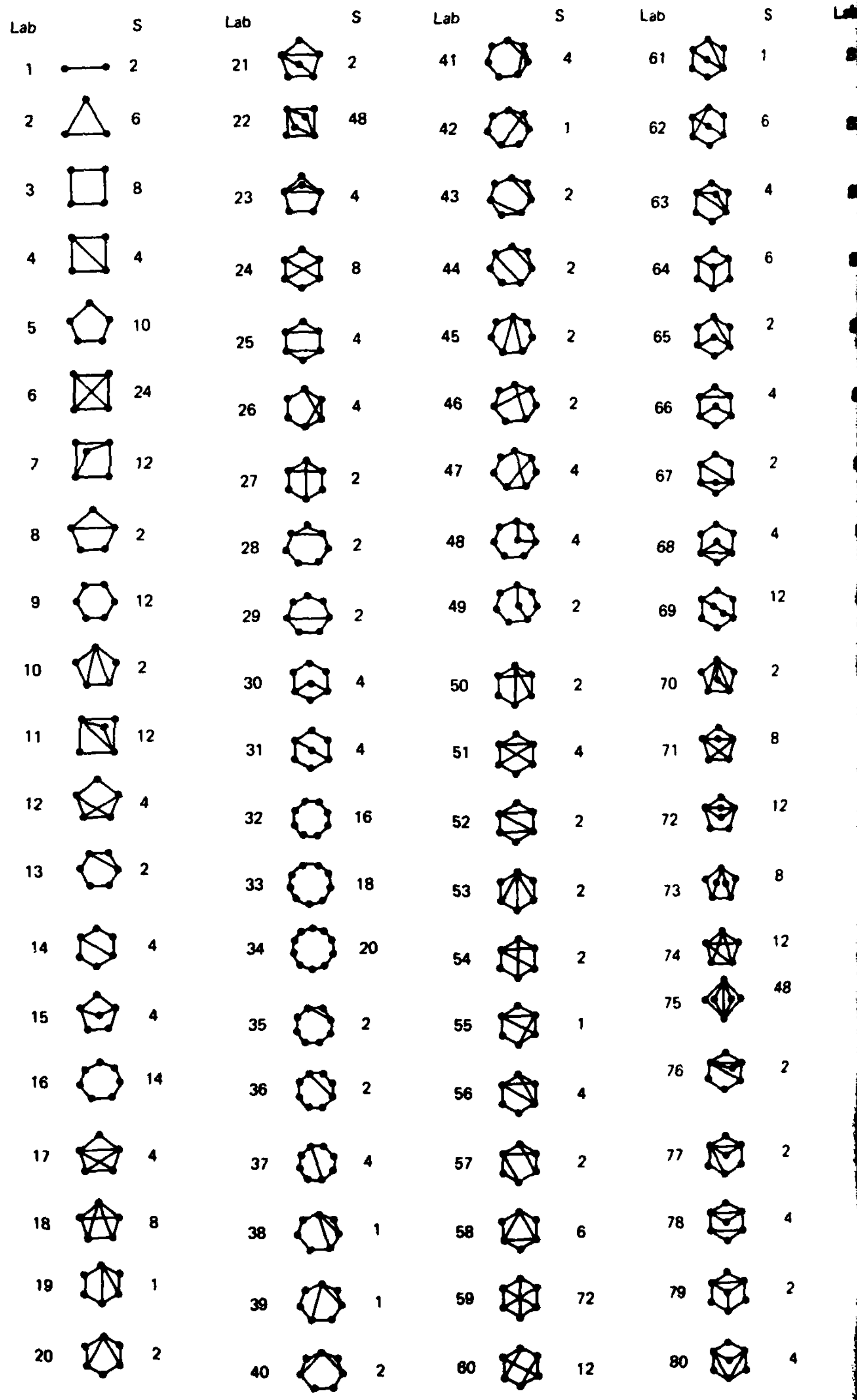
The program takes these data for a single-bonded diagram, generates the labels of the appropriate density weight factors, multiplies these NC polynomials together, and multiplies the result by the ratio of the free multiplicity divided by the symmetry number. The final result is then accumulated in the appropriate $C_{n,m}$, where

$$-\beta F = -L[\rho \ell n \rho + (1-\rho)\,\ell n(1-\rho)] + \sum_{n=1}^{10} \sum_{m=1}^{2n} C_{n,m}\,\rho^m (J/kT)^n + O[(J/kT)^{11}]. \quad (2)$$

Next, the program automatically multiple-bonds the diagram and repeats the procedure. The free energy series for the three cubic lattices are given in Tables 4 through 6. These coefficients were compared with the results available in the literature. In particular, for the simple-cubic and body-centered-cubic lattices, the low temperature series of Sykes, Essam, and Gaunt[11] were used to determine the high temperature series by means of an inversion of the activity series into a density series. For the face-centered-cubic lattice, McKenzie's recent results[12] for the low temperature series were inverted. Exact agreement is found in all cases. Thus, we are confident that the symmetry numbers and density weight factors are correct. The evaluation of Eq. 1 for more general models (e.g., longer ranged interactions, multiple sublattice long range order parameters, etc.) are under way.

[11] M. F. Sykes, J. W. Essam, and D. S. Gaunt, "Derivation of Low-Temperature Expansions for the Ising Model of a Fer romagnet and an Antiferromagnet," *J. Math. Phys.* **6**, 283 (1965).

[12] S. McKenzie, "Extended High Temperature Low Field Expansions for the Ising Model," *Can. J. Phys.* **57**, 1239 (1979).



Lab	S	Lab	S	Lab	S	Lab	S
1	2	21	2	41	4	61	1
2	6	22	48	42	1	62	6
3	8	23	4	43	2	63	4
4	4	24	8	44	2	64	6
5	10	25	4	45	2	65	2
6	24	26	4	46	2	66	4
7	12	27	2	47	4	67	2
8	2	28	2	48	4	68	4
9	12	29	2	49	2	69	12
10	2	30	4	50	2	70	2
11	12	31	4	51	4	71	8
12	4	32	16	52	2	72	12
13	2	33	18	53	2	73	8
14	4	34	20	54	2	74	12
15	4	35	2	55	1	75	48
16	14	36	2	56	4	76	2
17	4	37	4	57	2	77	2
18	8	38	1	58	6	78	4
19	1	39	1	59	72	79	2
20	2	40	2	60	12	80	4

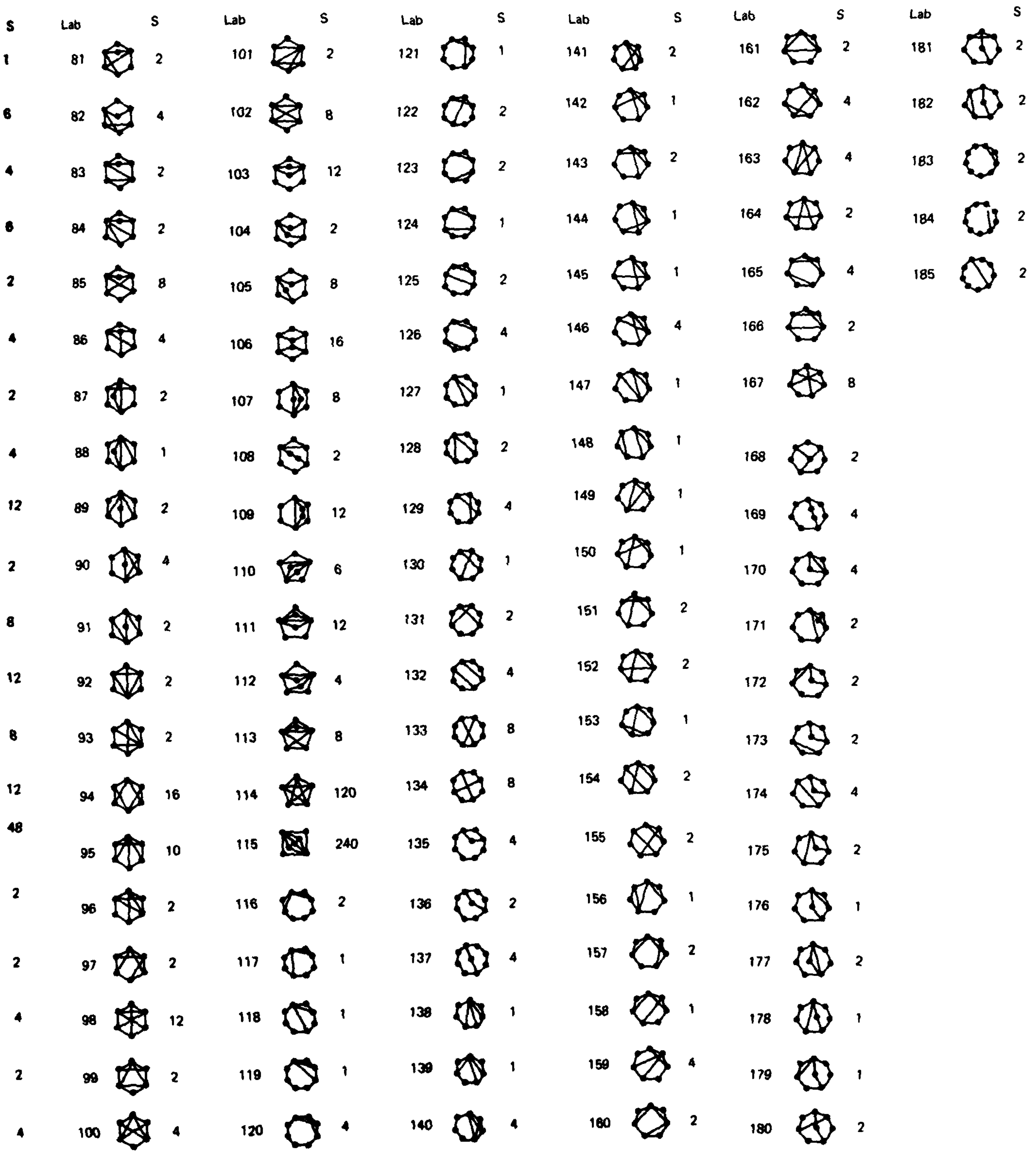


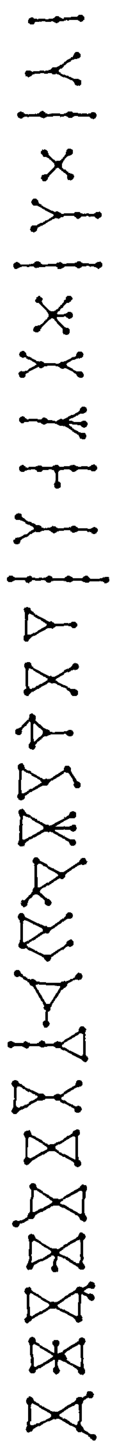
Figure 8—A complete list of more than simply connected diagrams with 10 or fewer bonds.

Table 2—The free multiplicities for the simple-cubic and body-centered-cubic lattices.

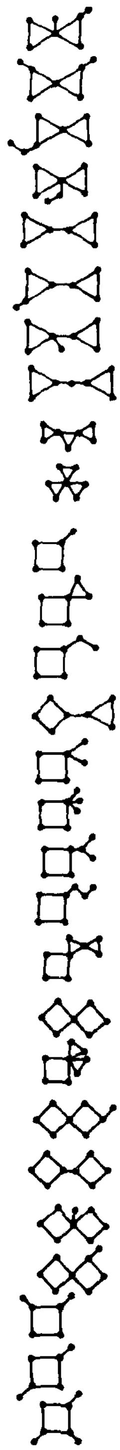
L	FM sc	FM bcc	L	FM sc	FM bcc
1	6	8	105	18612	140608
3	90	216	106	18612	140608
7	318	1000	109	20250	157464
9	1860	8000	115	8166	39304
14	1350	5832	128	20250	157464
22	1494	5832	129	18324	140608
24	960	4096	131	16134	125000
30	5712	32768	132	20250	157464
32	44730	343000	135	129330	1331000
34	1172556	16003008	137	108600	1124864
36	27900	216000	186	36	64
59	642	2744	187	216	512
64	3804	21952	188	216	512
67	4770	27000	189	1296	4096
69	22632	175616	190	1296	4096
85	4044	21952	191	1296	4096
86	3102	17576	192	7776	32768
103	24216	175616	193	7776	32768

Table 3—*The free multiplicities for the face-centered-cubic lattice.*

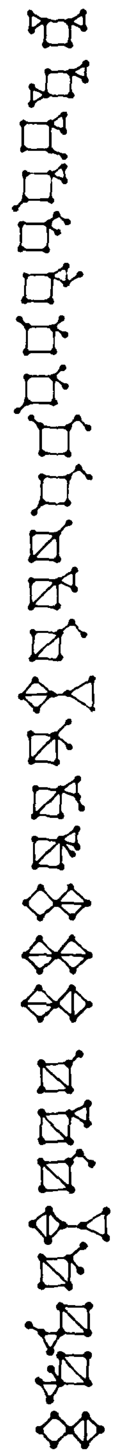
L	FM	L	FM	L	FM	L	FM	L	FM
1	12	38	69120	75	3072	112	49344	149	47520
2	48	39	97200	76	34560	113	768	150	48384
3	540	40	69120	77	34560	114	0	151	36336
4	192	41	66816	78	34560	115	268044	152	58752
5	4320	42	74304	79	35328	116	675840	153	35328
6	48	43	69120	80	49344	117	777600	154	58752
7	3084	44	97200	81	51360	118	777600	155	38064
8	2160	45	97200	82	28176	119	675840	156	34560
9	42240	46	83520	83	49344	120	602880	157	25920
10	768	47	102816	84	49344	121	688704	158	35328
11	768	48	1770240	85	107088	122	563760	159	36336
12	1056	49	1452096	86	75372	123	675840	160	34560
13	17280	50	2928	87	35328	124	777600	161	34560
14	24300	51	4224	88	34560	125	777600	162	28368
15	19728	52	3072	89	49344	126	675840	163	47520
16	403200	53	3072	90	42624	127	777600	164	37248
17	192	54	5136	91	49344	128	1093500	165	25920
18	384	55	4224	92	768	129	1015632	166	47520
19	8640	56	2160	93	1536	130	669888	167	47808
20	8640	57	4224	94	2976	131	838380	168	785088
21	12336	58	3072	95	960	132	1093500	169	13059648
22	25740	59	8412	96	1056	133	679536	170	675840
23	8640	60	3792	97	1776	134	567168	171	1110240
24	14688	61	78912	98	2592	135	17473500	172	783552
25	8640	62	59328	99	1536	136	13639680	173	783552
26	6480	63	97200	100	2976	137	13971072	174	887760
27	8832	64	104112	101	768	138	34560	175	887760
28	168960	65	78912	102	768	139	34560	176	783552
29	194400	66	78912	103	1361136	140	17280	177	777600
30	195888	67	138780	104	766512	141	36000	178	887760
31	155952	68	69120	105	978240	142	28128	179	623808
32	4038300	69	1468272	106	978240	143	25920	180	671904
33	40958400	70	3072	107	808704	144	25920	181	562176
34	423550512	71	8640	108	623808	145	35328	182	623808
35	1612800	72	130320	109	1093500	146	25920	183	16153200
36	1900800	73	90624	110	102960	147	34560	184	18144000
37	1555200	74	48	111	34560	148	34560	185	15206400



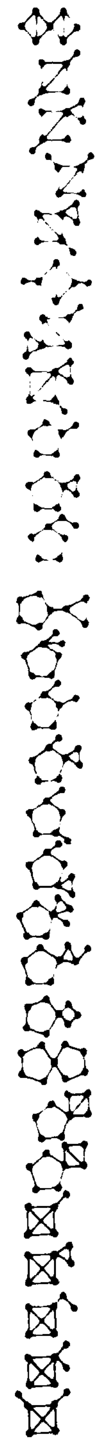
Lab	S
186	2
187	6
188	2
189	24
190	2
191	2
192	120
193	8
194	6
195	2
196	2
197	2
198	2
199	4
200	2
201	2
202	12
203	2
204	1
205	6
206	2
207	4
208	8
209	2
210	8
211	4
212	16
213	4



Lab	S
214	2
215	2
216	2
217	8
218	8
219	2
220	4
221	8
222	8
223	48
224	2
225	4
226	2
227	4
228	4
229	12
230	4
231	2
232	4
233	8
234	16
235	4
236	8
237	8
238	2
239	2
240	4
241	2



Lab	S
242	8
243	16
244	2
245	4
246	2
247	2
248	2
249	4
250	1
251	2
252	2
253	4
254	2
255	4
256	4
257	2
258	4
259	4
260	8
261	4
262	2
263	4
264	2
265	4
266	4
267	2
268	4
269	4



Lab	S
27[illegible]	[illegible]
[illegible]	4
272	[illegible]
273	[illegible]
274	[illegible]
275	4
276	4
[illegible]	2
278	2
279	4
280	2
281	4
282	4
283	2
284	2
285	2
286	2
287	4
288	2
289	4
290	8
291	4
292	4
293	6
294	12
295	6
296	12
297	4

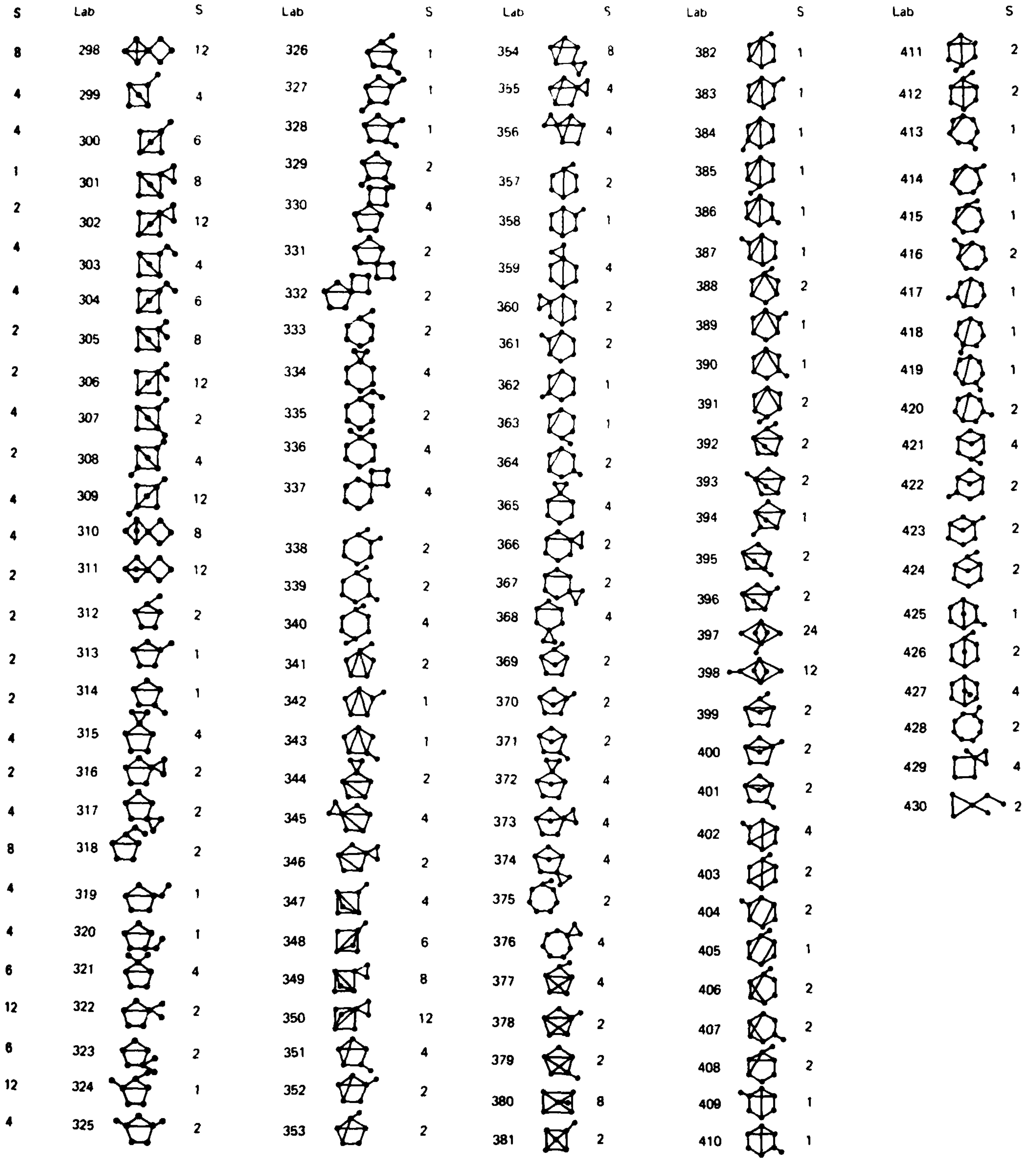


Figure 9—Articulated single-bonded diagrams with 10 or fewer bonds subject to the dumbbell rule.

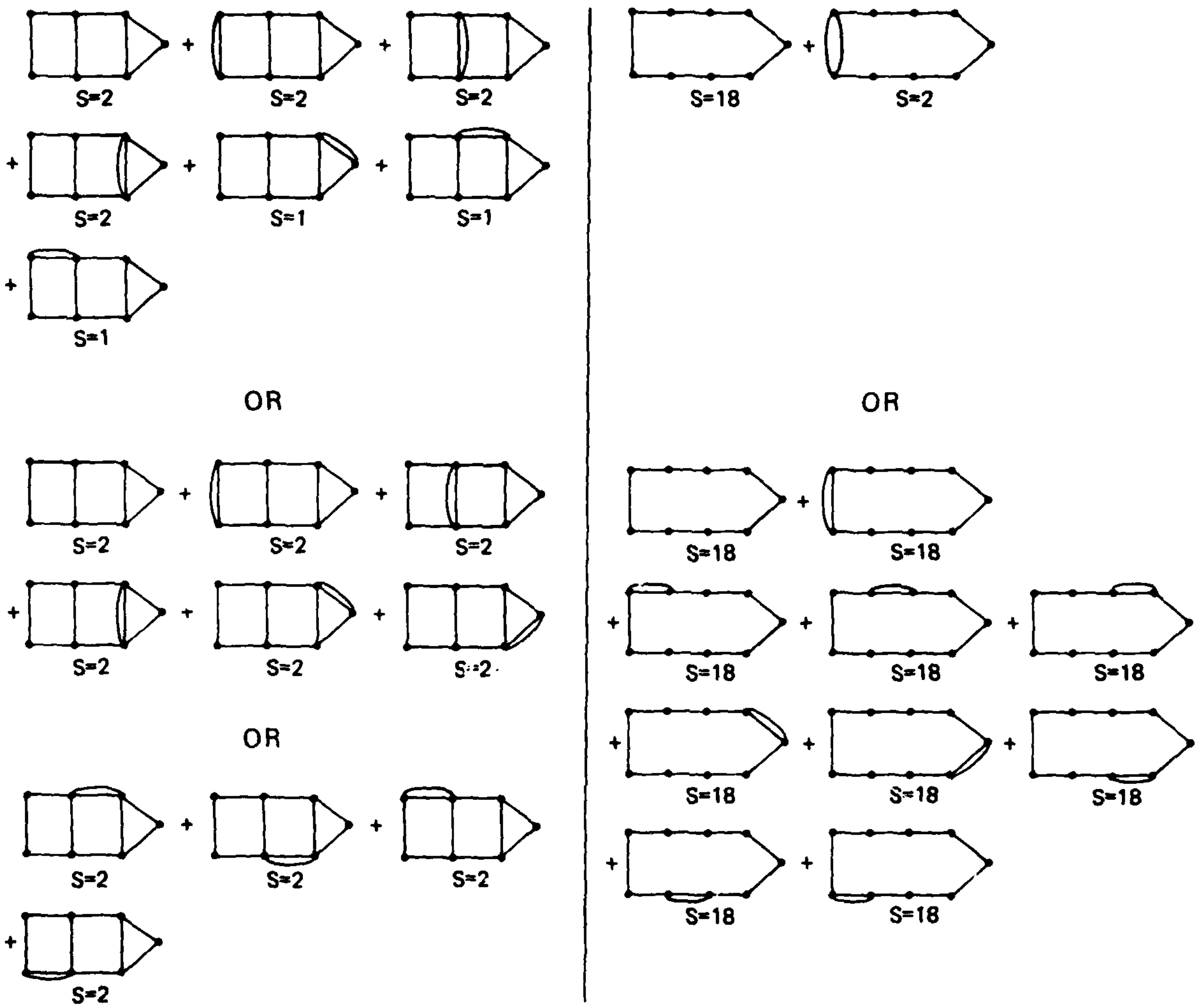


Figure 10—*Examples of the two alternate ways of multiple-bonding a diagram.* (As discussed in the text, the first method uses only topologically distinct diagrams and their associated symmetry numbers. The alternative procedure, which was used, does the multiple-bonding independently and uses only the symmetry number of the single-bonded diagram. The advantage of this alternative is that it is trivial to implement on the computer.)

Table 4—The coefficients of $\rho^k (\beta J)^n$ in the Taylor-series expansion of the Helmholtz free energy of the nearest-neighbor lattice gas on the face-centered-cubic lattice. The entry $C(n,k) = ij{:}lm$ is to be read as $ij + [lm/(n!2)]$, e.g., $C(9,8) = 21591{:}498960 = 215291 + 498960/(9!2) = 215291.6875$.

k↓/n→	1	2	3	4	5	6	7	8	9	10
2	6:0	3:0	1:0	0:12	0:12	0:12	0:12	0:12	0:12	0:12
3	0:0	-6:0	2:0	8:24	8:120	5:696	2:7224	1:9048	0:284280	0:883416
4	0:0	3:0	-11:0	-34:12	-10:180	49:372	96:588	104:66036	84:613740	56:615252
5	0:0	0:0	12:0	57:0	-75:0	-374:720	-394:7056	158:17136	1042:344880	1765:2409840
6	0:0	0:0	-4:0	-54:0	285:96	1021:0	-149:4368	-4336:14112	-7039:495984	-1184:5724000
7	0:0	0:0	0:0	30:0	-468:0	-1495:0	4542:0	16482:30240	-6581:181440	-114154:5320800
8	0:0	0:0	0:0	-7:24	423:0	1225:1080	-14813:7920	-21321:7560	215291:498960	916676:3870360
9	0:0	0:0	0:0	0:0	-204:0	-480:0	26854:0	-33913:40320	-1119307:544320	-4000948:3628800
10	0:0	0:0	0:0	0:0	40:192	8:0	-31784:0	193247:0	3419749:84672	11978410:4596480
11	0:0	0:0	0:0	0:0	0:0	48:0	25452:0	-393420:0	-7211599:0	-26568250:1451520
12	0:0	0:0	0:0	0:0	0:0	-8:0	-13446:0	476890:0	11052791:362880	45108674:5564160
13	0:0	0:0	0:0	0:0	0:0	0:0	4248:0	-371007:0	-12494314:0	-59478333:0
14	0:0	0:0	0:0	0:0	0:0	0:0	-606:8640	182406:0	10350458:0	61194742:0
15	0:0	0:0	0:0	0:0	0:0	0:0	0:0	-51762:0	-6122232:0	-48994063:4354560
16	0:0	0:0	0:0	0:0	0:0	0:0	0:0	6470:20160	2450285:0	30169646:1088640
17	0:0	0:0	0:0	0:0	0:0	0:0	0:0	0:0	-594708:0	-13920714:0
18	0:0	0:0	0:0	0:0	0:0	0:0	0:0	0:0	66078:483840	4565694:0
19	0:0	0:0	0:0	0:0	0:0	0:0	0:0	0:0	0:0	-953352:0
20	0:0	0:0	0:0	0:0	0:0	0:0	0:0	0:0	0:0	95335:1451520

Table 5—The coefficients of $\rho^k (\beta J)^n$ in the Taylor-series expansion of the Helmholtz free energy of the nearest-neighbor lattice gas on the body-centered cubic lattice.

k↓/n→	1	2	3	4	5	6	7	8	9	10
2	4:0	0:8	0:8	0:8	0:8	0:8	0:8	0:8	0:8	0:8
3	0:0	-4:0	-4:0	-2:16	-1:0	-0:496	-0:1008	-0:2032	-0:4080	-0:8176
4	0:0	2:0	8:8	23:8	32:200	31:248	22:4424	13:9752	6:365000	2:5879768
5	0:0	0:0	-8:0	-74:0	-230:0	-368:480	-390:2016	-306:74592	-189:673440	-94:5503200
6	0:0	0:0	2:8	104:0	716:224	2070:960	3631:6272	4599:51072	4630:64544	3934:3004800
7	0:0	0:0	0:0	-68:0	-1192:0	-6523:480	-19593:3360	-39780:68544	-60576:201600	-73531:2212800
8	0:0	0:0	0:0	17:0	1102:0	12336:1200	64691:4800	209144:17136	471586:110880	801956:4242480
9	0:0	0:0	0:0	0:0	-536:0	-14353:480	-136674:6720	-709859:26880	-2376364:524160	-5687290:2217600
10	0:0	0:0	0:0	0:0	107:48	10086:960	189061:3360	1620446:53760	8157048:459648	27714932:927360
11	0:0	0:0	0:0	0:0	0:0	-3936:0	-170832:0	-2543142:0	-19688292:0	-96122683:1451520
12	0:0	0:0	0:0	0:0	0:0	656:0	97320:0	2755277:0	34019431:241920	242926042:967680
13	0:0	0:0	0:0	0:0	0:0	0:0	-31776:0	-2028222:0	-42324389:241920	-453899786:0
14	0:0	0:0	0:0	0:0	0:0	0:0	4539:4320	969876:0	37643736:0	630878500:0
15	0:0	0:0	0:0	0:0	0:0	0:0	0:0	-272052:0	-23371461:241920	-650529826:2903040
16	0:0	0:0	0:0	0:0	0:0	0:0	0:0	34006:40320	9629247:241920	491061591:725760
17	0:0	0:0	0:0	0:0	0:0	0:0	0:0	0:0	-2367464:0	-263758596:0
18	0:0	0:0	0:0	0:0	0:0	0:0	0:0	0:0	263051:403200	95496836:0
19	0:0	0:0	0:0	0:0	0:0	0:0	0:0	0:0	0:0	-20902208:0
20	0:0	0:0	0:0	0:0	0:0	0:0	0:0	0:0	0:0	2090220:5806080

Table 6—The coefficients of $\rho^k (\beta J)^n$ in the Taylor-series expansion of the Helmholtz free energy of the nearest-neighbor lattice gas on the simple cubic lattice.

k↓/n→	1	2	3	4	5	6	7	8	9	10
2	3:0	0:6	0:6	0:6	0:6	0:6	0:6	0:6	0:6	0:6
3	0:0	-3:0	-3:0	-1:36	-0:180	-0:372	-0:756	-0:1524	-0:3060	-0:6132
4	0:0	1:2	6:6	11:18	12:150	10:546	6:8358	3:61746	1:576150	0:5473986
5	0:0	0:0	-6:0	-31:24	-76:120	-113:360	-119:6552	-98:51912	-67:21240	-38:6660360
6	0:0	0:0	2:0	42:0	225:168	603:0	1029:7224	1288:2016	1277:653208	1057:3679200
7	0:0	0:0	0:0	-27:0	-366:0	-1828:720	-5123:0	-9712:67536	-13853:393120	-15864:5190480
8	0:0	0:0	0:0	6:36	334:120	3374:900	15927:6120	46134:6804	94372:325080	148380:1978020
9	0:0	0:0	0:0	0:0	-162:0	-3870:0	-32313:0	-145814:20160	-431292:90720	-933449:907200
10	0:0	0:0	0:0	0:0	32:96	2699:0	43548:0	316910:60480	1377987:102816	4140755:6683040
11	0:0	0:0	0:0	0:0	0:0	-1050:0	-38730:0	-481078:40320	-3156709:362880	-13354439:3084480
12	0:0	0:0	0:0	0:0	0:0	175:0	21873:0	509881:60480	5253431:544320	31931785:756000
13	0:0	0:0	0:0	0:0	0:0	0:0	-7116:0	-370198:40320	-6365135:0	-57232551:3628800
14	0:0	0:0	0:0	0:0	0:0	0:0	1016:5760	175653:0	5559771:0	77139645:0
15	0:0	0:0	0:0	0:0	0:0	0:0	0:0	-49107:0	-3411756:0	-77794745:5806080
16	0:0	0:0	0:0	0:0	0:0	0:0	0:0	6138:30240	1396200:362880	57820459:2358720
17	0:0	0:0	0:0	0:0	0:0	0:0	0:0	0:0	-342258:0	-30740634:0
18	0:0	0:0	0:0	0:0	0:0	0:0	0:0	0:0	38028:483840	11063145:0
19	0:0	0:0	0:0	0:0	0:0	0:0	0:0	0:0	0:0	-2415006:0
20	0:0	0:0	0:0	0:0	0:0	0:0	0:0	0:0	0:0	241500:4354560

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APPENDIX

THE COMPILATION PROGRAM

The notations used in this computer program are:

I	Diagram label.
S	Symmetry number.
W	Free multiplicity.
NB	Number of connected vertex pairs.
L → L(10); L(1), L(2), ...,L(NB)	The lower limit on the number of bonds between, respectively, the first, second, ..., and *NB*th vertex pair.
INSLUM	The number of bonds in the single-bonded diagram.
NC	The number of vertices (circles).
JAO → JAO(NC); JAO(1), JAO(2) ..., JAO(NC)	The articulation orders of, respectively, the first, second, ..., and *NC*th vertex.
JAOSUM	The number of indices that must be specified in the product of polynomials (*M*'s).
NNN	Specifies the vertex label unless one (or more) of the vertices (say the *j*th) is articulated, in which case $jao(j)$ of the *NNN's* are used for it and all subsequent labels are $[jao(j) - 1]$ out of sync. (This concept is illustrated below.)
NP →(5,NNN)	Specifies the bonds that emanate from the vertex labeled by *NNN*. (Again, see below.)
IIT	Specifies the total number of bonds that can be added to a single-bonded diagram.
IjT	Specifies the upper limit on the number of bonds between the *j*th vertex pair.
INL →	$L(N)$.

Figures A-1 and A-2 illustrate these conventions for two representative articulated diagrams.

Lines 2 through 59 of the main program read in the data, identify the topology of the single-bonded diagram and prepare the do-loops to be used in multiple bonding. The integers $j_1, j_2, \ldots, j_{NB}$ generated in lines 61 through 125 specify, respectively, the number of bonds between the first, the second,..., and the *NB*th vertex pairs. Lines 126 through 168 obtain the indices, $N(III)$, for each of the circles, *III*; identify the corresponding density weight factors; and multiplies them together. The multiplication of these polynomials is accomplished in a subroutine, POLYMT, which is also listed. Steps 169 through 214 accumulate the contributions to the coefficients $C_{n,m}$ of Eq. 2.

The following pages list the compilation program.

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```
C     EVALUATES ARTICULATION ISING DIAGRAMS.      S FAVIN   AUG 1982
      IMPLICIT REAL*16(A-H,O-Z)
      DIMENSION P(11,3,3,4,6,11), L(10), I(10), S1(21)
      DIMENSION NP(5,10),   JAO(10), N(5)
      DIMENSION SS1(21,11)
      DIMENSION ZZ(26136)
       COMMON    DEBUG
      LOGICAL DEBUG
      EQUIVALENCE (P(1,1,1,1,1,1), ZZ(1))
      EQUIVALENCE (N(1),N1), (N(2),N2), (N(3),N3), (N(4),N4), (N(5),N5)
      EQUIVALENCE (L(1),I1L), (L(2),I2L), (L(3),I3L), (L(4),I4L),
     1  (L(5),I5L), (L(6),I6L), (L(7),I7L), (L(8),I8L), (L(9),I9L),
     2   (L(10),I10L)
      DATA SS1 /231*0.0Q0/
      DATA   L/10*0/,   I/10*0/
C
C     DEBUG = .TRUE.
C     DEBUG = .FALSE.
      DEBUG = .FALSE.
      DO 3 K=1,26136
    3 ZZ(K) = 0.0D0
      CALL READIN( P )
C
C     28-ELEMENTAL (SINGLE-BONDED) DIAGRAMS
      PRINT 17
C
      DO 100 J=1,430
      IF(DEBUG)  PRINT 17
   17 FORMAT('1')
      READ (5,1,END=101)   S,W,NB,NC,L
    1 FORMAT(2F10.0,12I2)
      PRINT 2, J, S, W, NB, NC, L
    2 FORMAT(I4,2F16.1,2I6,3X,10I3)
      IF(S .EQ. 0.0D0) GO TO 789
C
      INLSUM = 0
      DO 15 M=1,NB
      INLSUM = INLSUM + L(M)
   15 CONTINUE
C     MOW CHECK ON NC 1"S IN JAO
C
      READ 5,JAO
    5 FORMAT(10I2)
C     IF(DEBUG) PRINT 6, (JAO(M),M=1,NC)
                PRINT 6, (JAO(M),M=1,NC)
```

```
    6 FORMAT('0  JAO: ',10I4)
      JAOSUM = 0
      DO 16 M=1,NC
      JAOSUM = JAOSUM + JAO(M)
   16 CONTINUE
C     IF(DEBUG) PRINT 7, JAOSUM
                PRINT 7, JAOSUM
    7 FORMAT('           JAO_SUM IS ',I5)
C
C     ASSUME JAOSUM > 0
      DO 18 NNN=1,JAOSUM
      READ 5, (NP(JJ,NNN),JJ=1,5)
C     IF(DEBUG) PRINT 8, NNN, (NP(JJ,NNN),JJ=1,5)
                PRINT 8, NNN, (NP(JJ,NNN),JJ=1,5)
   18 CONTINUE
    8 FORMAT(I5,5I3)
C
C
C
C
      IIT = 10 - INLSUM
      I1T = IIT + I1L
      I2T = IIT + I2L
       I3T = IIT + I3L
        I4T = IIT + I4L
         I5T = IIT + I5L
          I6T = IIT + I6L
           I7T = IIT + I7L
            I8T = I1T + I8L
             I9T = I1T + I9L
              I10T = I1T + I10L
   10 FORMAT('0 IIT=',I5,5X,'I1T,...I10T=',10I5)
      IF(DEBUG)
     *PRINT 10, IIT, I1T,I2T,I3T,I4T,I5T,I6T,I7T,I8T,I9T,I10T
C
      DO 90 I1=I1L, I1T
      I(1)=I1
      IF(NB .EQ. 1) GO TO 999
       DO 88 I2=I2L, I2T
       J2 = I2 + I1
       IF(J2 .GT. 10) GO TO 90
       I(2) = I2
       IF(NB .EQ. 2) GO TO 999
        DO 86 I3=I3L, I3T
        J3 = J2 + I3
```

```
      IF(J3 .GT. 10) GO TO 88
      I(3) = I3
      IF(NB .EQ. 3) GO TO 999
       DO 84 I4=I4L, I4T
       J4 = J3 + I4
       IF(J4 .GT. 10) GO TO 86
       I(4) = I4
       IF(NB .EQ. 4) GO TO 999
        DO 82 I5=I5L, I5T
        J5 = J4 + I5
        IF(J5 .GT. 10) GO TO 84
        I(5) = I5
        IF(NB .EQ. 5) GO TO 999
         DO 80 I6=I6L, I6T
         J6 = J5 + I6
         IF(J6 .GT. 10) GO TO 82
         I(6) = I6
         IF(NB .EQ. 6) GO TO 999
          DO 78 I7=I7L, I7T
          J7 = J6 + I7
          IF(J7 .GT. 10) GO TO 80
          I(7) = I7
          IF(NB .EQ. 7) GO TO 999
           DO 76 I8=I8L,I8T
           J8=J7+I8
           IF(J8 .GT. 10) GO TO 78
           I(8) = I8
           IF(NB .EQ. 8) GO TO 999
            DO 74 I9=I9L,I9T
            J9 = J8 + I9
            IF(J9 .GT. 10) GO TO 76
            I(9) = I9
            IF(NB .EQ. 9) GO TO 999
             DO 72 I10=I10L, I10T
             J10 = J9 + I10
             IF(J10 .GT. 10) GO TO 74
             I(10) = I10
C
C
C
C
C
  999       F = S
    IF(DEBUG)
   *PRINT 12, I1, I2, I3, I4, I5, I6, I7, I8, I9, I10
```

```
   12 FORMAT('0  I1,...,I10= ',10I5)
            DO 20 K=2,21
   20       S1(K) = 0.0D0
            S1(1) = 1.0D0
         NS1 = 1
         NNN=0
         DO 30 II=1,NC
         IAO = JAO(II)
          DO 29 III=1,5
   29     N(III)=0
           DO 27 III = 1, IAO
           NNN=NNN+1
             DO 26 JJ=1,5
             KK=NP(JJ,NNN)
             IF(KK .LE.0) GO TO 27
             N(III) = N(III) + I(KK)
   26        CONTINUE
   27      CONTINUE
C
C     NOW ORDER THE N(I) AND MULT S1 * P(N, N1+1, N2+1, N3+1)
C
C
           DO 35 IN=1,4
           IS=IN+1
               DO 35 JN=IS,5
               IF(N(IN) .LE. N(JN)) GO TO 35
               NSAVE = N(IN)
               N(IN) = N(JN)
               N(JN) = NSAVE
   35      CONTINUE
      IF(DEBUG)  PRINT 11, N
   11 FORMAT(' SORT N IS ',5I5)
           N11 = N1+1
           N21= N2+1
           N31= N3+1
           N41= N4+1
           N51= N5+1
C
      NN1 = N1 + N2 + N3 + 1 + N4 + N5
      CALL POLYMT(P(1,N11, N21, N31, N41, N51), NN1, S1, NS1, S1)
      NS1 = NS1+NN1-1
   30    CONTINUE
C
C
C
```

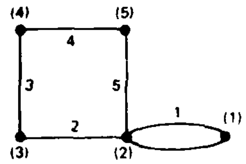
```
C
C
            KK=0
            F=S
            DO 40 K=1,NB
                  FACT = 1.0D0
                  IFK = I(K)
                  DO 28 IFF=1,IFK
   28             FACT = FACT * IFF
            F = F * FACT
         IF(DEBUG)
        *PRINT 9, NB,NC,I,   F
    9 FORMAT(' FACT:',2I6,10I3,1PG20.12 )
   40       KK = KK + I(K)
         IF(KK .GT. 0) GO TO 49
         PRINT 13, I
   13 FORMAT('1****ERROR KK=0 AND I=',10I5)
         STOP
C
   49 CONTINUE
         KZ=1
            DO 50 K=1,21
            SS1(K,KK) = SS1(K,KK) + W*S1(K)/F
            IF(SS1(K,KK) .NE. 0.0D0) KZ=K
   50       CONTINUE
C
C        IF(J .GT. 3) GO TO 60
C
C    4 FORMAT(' KK=',I5,1P5G20.12,/,(1P6G20.12))
C        IF(DEBUG) PRINT 4, KK, (SS1(K,KK),K=1,KZ)
                   PRINT 4, KK, (SS1(K,KK),K=1,KZ)
    4 FORMAT(' KK=',I5,/,(1P5G26.16))
   60 CONTINUE
         GO TO (90, 88, 86, 84, 82, 80, 78, 76, 74, 72), NB
C
   72             CONTINUE
   74            CONTINUE
   76           CONTINUE
   78          CONTINUE
   80         CONTINUE
   82        CONTINUE
   84       CONTINUE
   86      CONTINUE
   88     CONTINUE
   90 CONTINUE
```

```
  100 CONTINUE
  101 CONTINUE
      DO 954 KK=1,11
      PRINT 4, KK, (SS1(K,KK),K=1,21)
      PUNCH 25,(SS1(K,KK),K=2,21)
  25  FORMAT(1P3G26.16)
  954 CONTINUE
  789 CONTINUE
      STOP
      END
```

```
      SUBROUTINE READIN ( P )
      IMPLICIT REAL*16(A-H,O-Z)
C
      DIMENSION P(11,3,3,4,6,11), IP(5)
      EQUIVALENCE (IP(1),N), (IP(2),L), (IP(3),K), (IP(4),J), (IP(5),I)
C
      PRINT 1
    1 FORMAT('1 READIN P(M,N,L,K,J,I),M=2,11)',//)
      DO 100 IR=1,100
      READ (9,4) IP
    4 FORMAT(5I3)
      IF(N .EQ. 0) GO TO 90
      READ(9,5)  (P(M,N,L,K,J,I),M=2,11)
      PRINT 6, N, L, K,J,I, (P(M,N,L,K,J,I),M=2,11)
    6 FORMAT('0',5I5,5F13.2,/,(25X,5F13.2))
  100 CONTINUE
      IR=101
C
   90    CONTINUE
      IR=IR-1
      PRINT 3, IR
    3 FORMAT('0  ',I5,' CARDS WERE READIN INTO POLY')
    5 FORMAT(10F8.0)
       PRINT 2
    2  FORMAT('1')
      RETURN
      END
```

```
      SUBROUTINE POLYMT(P, NP, S, NS, A)
      IMPLICIT REAL*16(A-H,O-Z)
      DIMENSION P(NP), S(NS), A(21), B(21)
       COMMON    DEBUG
      LOGICAL DEBUG
C
C     DEBUG = .TRUE.
C     DEBUG = .FALSE.
      IF(DEBUG) PRINT 1, NP, (P(I),I=1,11)
      IF(DEBUG) PRINT 2, NS, (S(I),I=1,21)
    1 FORMAT(' INPUT P POLY  NP=',I5, //,(1P5G20.12) )
    2 FORMAT(' INPUT S POLY  NS=',I5, //,(1P5G20.12) )
    3 FORMAT(' OUTPUT THE B POLY',//,(1P5G20.12) )
C
      DO 10 I=1,21
   10 B(I) = 0.0D0
C     ASSUME NP .GE. 2
      IF(NS .GT. 1) GO TO 20
C     SPECIAL FOR NS=1
      DO 15 L=1,NP
   15 B(L) = S(1) * P(L)
C
C     GENERAL RETURN
C
   99 CONTINUE
      IF(DEBUG) PRINT 3, B
      DO 100 L=1,21
      A(L) = B(L)
  100 CONTINUE
      RETURN
C
C
   20 CONTINUE
      IF(NP .GT. NS) GO TO 40
C     FOR NP .LE. NS
      NP1 = NP-1
      DO 30 L=1,NP1
      LP1 = L+1
      DO 30 I=1,L
      B(L) = B(L) + P(I) * S(LP1-I)
   30 CONTINUE
C
      DO 33 L=NP,NS
      LP1 = L+1
      DO 33 I=1,NP
```

```
      B(L) = B(L) + P(I) * S(LP1-I)
   33 CONTINUE
C
      NPNS = NP+ NS
      NS1 = NS+1
      N2 = NPNS - 1
      DO 36 L=NS1, N2
      LNS = L - NS
      I1 = NPNS - L
      DO 36 I=1,I1
      B(L) = B(L) + P(LNS+I) * S(NS1 - I)
   36 CONTINUE
      GO TO 99
C
C
C     NP .GT. NS
   40 CONTINUE
      NS1 = NS-1
      DO 50 L=1,NS1
      LP1 = L+1
      DO 50 I=1,L
      B(L) = B(L) + S(I) * P(LP1 - I)
   50 CONTINUE
C
      DO 53 L=NS, NP
      LP1 = L+1
      DO 53 I=1,NS
      B(L) = B(L) + S(I) * P(LP1 - I)
   53 CONTINUE
C
      NP1 = NP+1
      NPNS = NS + NP
      N2 = NPNS - 1
      DO 56 L=NP1, N2
      LNS = NPNS - L
      NPL = L-NP
      DO 56 I=1,LNS
      B(L) = B(L) + S(NPL+I) * P(NP1 - I)
   56 CONTINUE
      GO TO 99
      END
```



(p) labels the vert[illegible]s

i labels the bond

S = 2

W = { 6480 for f.c.c.; 540 for s.c; 1728 for b.c.c

NB = 5

L = (2, 1, 1, 1 1, 0, 0, 0, 0, 0)

INSLUM = 6

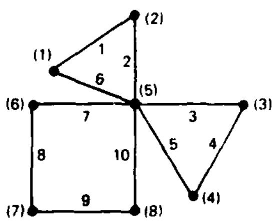
NC = 5

JAO = (1 2, 1 1, 1, 0, 0, 0, 0, 0)

JAOSUM = 6

Circle	NNN	NP
(1)	1	1, 0 0, 0, 0
(2)	2	1, 0, 0, 0, 0
	3	2, 5, 0, 0 0
(3)	4	2, 3, 0, 0, 0
(4)	5	3, 4, 0, 0, 0
(5)	6	4, 5, 0, 0, 0
	IIT =	4
	I1T =	6
	I2T =	5
	I3T =	5
	I4T =	5
	I5T =	5

Figure A-1—An illustration of the notations used in the main program. (The diagram's symmetry number does not account for the interchangeability of multiple bonds between a connected pair of vertices.)



(p) labels the vertices

i labels the bond

S = 16

W = { 1, 244, 160 for f.c.c.; 0 for s.c.; 0 for b.c.c.

NB = 10

L = (1, 1, 1; 1, 1, 1, 1, 1, 1, 1)

INSLUM = 10

NC = 8

JAO = (1, 1, 1, 1, 3, 1, 1, 1, 0, 0)

JAOSUM = 10

Circle	NNN	NP
(1)	1	1, 6, 0, 0, 0
(2)	2	1, 2, 0, 0, 0
(3)	3	3, 4, 0, 0, 0
(4)	4	4, 5, 0, 0, 0
(5)	5	2, 6, 0, 0, 0
	6	3, 5, 0, 0, 0
	7	5, 6, 0, 0, 0
(6)	8	7, 8, 0, 0, 0
(7)	9	8, 9, 0, 0, 0
(8)	10	9, 10, 0, 0, 0

Figure A-2—An example of the notation used in the main program

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The work reported in TG 1337 was done under Navy Contract N00024-83-C-5301. This work is supported by the Naval Sea Systems Command.

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